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What Is Claimed Is:

1. A method for evaluating the ability of a compound to associate with a molecule or molecular complex comprising a human serum albumin binding region selected from the group consisting of binding subdomains IA, IA/IB, IA/IIA, IB, I/II; I/III; II/III, IIA, IIA/IIB, IIB, IIIA, IIIA/IIIB, IIIB and IIIB', said method comprising the steps of:

a) constructing a computer model of said binding region defined by three-dimensional structural binding coordinates wherein the root mean square deviation between said structural binding coordinates and the structural binding coordinates of the resulting complex within the binding region as set forth in Table II or III is not more than about 1.15 angstroms;

b) selecting a compound to be evaluated by a method selected from the group consisting of (i) assembling molecular fragments into said compound, (ii) selecting a compound from a small molecule database, (iii) de novo ligand design of said compound, (iv) a compound obtained by modifying a compound with known binding affinity to a human serum albumin binding region; (v) a pharmaceutical or other compound as set forth in Tables I or II; (vi) a compound obtained by modifying a known pharmaceutical compound, or active portion thereof, of human serum albumin

c) employing computational means to perform a fitting program operation between computer models of the said compound to be evaluated and said binding region in order to provide an energy-minimized configuration of the said compound in the binding region; and

d) evaluating the results of said fitting operation to quantify the association between the said compound and the binding region computer model, thereby evaluating the ability of the said compound to associate with the said binding region.

2. The method of claim 1 wherein the root mean square deviation is within about 2.5 angstroms.

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3. The method of claim 1 wherein the root mean square deviation is within about 3.0 angstroms.

4. The method of claim 1 wherein the psi angle is in the range of about –
5   30 degrees. to +30 degrees

5. The method of claim 1 wherein the .phi. angle is in the range of about 60 degrees to 120.degrees.

10   6. The method of Claim 1 wherein the human serum albumin binding subdomain is binding region 1B, and wherein the three-dimensional structural binding coordinates at positions F036, F037, D108, P110, N111, L112, P113, R114, L115, V116, R117, P118, V122, M123, A126, N130, T133, F134, L135, K137, Y138, L139, Y140, E141, I142, A143, R145, H146, P147, Y148, F149,
15   Y150, L154, F157, A158, Y161, F165, L182, D183, L185, R186, D187, G189, K190, K190, S192, S193, A194, Q196, R197, E425, Q459, and a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15 angstroms, are used to generate said three-dimensional structure of said binding region defined by three-dimensional structural binding coordinates.
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7. The method of Claim 6 wherein the compound to be evaluated is a compound binding to the IB subdomain having three dimensional structural coordinates at the positions shown in Tables I and II.

25   8. The method of Claim 1 wherein the human serum albumin binding subdomain is binding region IIA, and wherein the three-dimensional structural binding coordinates at positions F149, Y150, E153, A191, S192, K195, Q196, L198, K199, C200, S202, F211, W214, A215, R218, L219, R222, F223, L234, L238, V241, H242, C245, C246, C253, D256, R257, L260, A261, I264, K286,
30   S287, H288, I290, A291, E292, V293, V343, P447, D451, Y452, V455, and a root mean square deviation from the backbone atoms of said amino acids of not

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more than 1.15 angstroms are used to generate said three-dimensional structure of said binding region defined by three-dimensional structural binding coordinates.

5   9. The method of Claim 8 wherein the compound to be evaluated is a compound binding to the IIA subdomain having three dimensional structural coordinates at the positions as shown in Tables I and II

         10. The method of Claim 1 wherein the human serum albumin binding
10   subdomain is binding region IIIA, and wherein the three-dimensional structural binding coordinates at positions E383, P384, K387, L387, I388, Q390, A391, N391, C392, F395, F403, L407, L408, R410, Y411, K414, V415, V418, T422, L423, V424, V426, S427, L430, G431, V433, G434, S435, C437, C438, R445, M446, A449, E450, W450, Y452, L453, V456, L457, L460, V473, R484, R485,
15   F488, S489, A490, L491, W492, and a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15 angstroms are used to generate said three-dimensional structure of said binding region defined by three-dimensional structural binding coordinates.

20   12. The method of Claim 10 wherein the compound to be evaluated is a compound binding to the IIIA subdomain having three dimensional structural coordinates at the positions shown in Tables I and II.

         13. The method of Claim 1 wherein the human serum albumin binding
25   subdomain is binding region IA, and wherein the three-dimensional structural binding coordinates at positions V007, F019, V023, F027, E045, V046, F049, A050, E060, N061, K064, L066, L069, F070, G071, D072, K073, C075, T076, C091, R098, L251, and a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15 angstroms are used to generate said
30   three-dimensional structure of said binding region defined by three-dimensional structural binding coordinates.

14. The method of Claim 13 wherein the compound to be evaluated is a compound binding to the IA subdomain having three dimensional structural coordinates at the positions shown in Tables I and II.

15. The method of Claim 1 wherein the human serum albumin binding subdomain is binding region IIA-IIB, and wherein the three-dimensional structural binding coordinates at positions L198, K199, S202, F206, R209, A210, F211, K212, A213, W214, V216, F228, V231, S232, D324, V325, L327, G328, L331, V343, V344, L347, A350, K351, E354, D451, S454, E479, S480, L481, V482, N483 and a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15 angstroms are used to generate said three-dimensional structure of said binding region defined by three-dimensional structural binding coordinates.

16. A method for identifying an activator or inhibitor of a molecule comprising a human serum albumin binding region selected from the group consisting of binding region IA, IA/IB, IA/IIA, IB, I/II; I/III; II/III, IIA, IIA/IIB, IIB, IIIA, IIIA/IIIB, IIIB and IIIB' comprising the steps of

a) constructing a computer model of the binding region defined by three-dimensional structural binding coordinates wherein the root mean square deviation between said structural binding coordinates and the structural binding coordinates of the resulting complex within the binding region as set forth in Table II or III is not more than about 1.15 angstroms;

b) selecting a compound to be evaluated by a method selected from the group consisting of (i) assembling molecular fragments into said compound, (ii) selecting a compound from a small molecule database, (iii) de novo ligand design of said compound, (iv) a compound obtained by modifying a compound with known binding affinity to a human serum albumin binding region; (v) a pharmaceutical or other compound as set forth in Tables I or II; (vi) a compound

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obtained by modifying a known pharmaceutical compound, or active portion thereof, of human serum albumin

c) employing computational means to perform a fitting program operation between computer models of the said compound to be evaluated and said
5   binding region in order to provide an energy-minimized configuration of the said compound in the binding region;

d) evaluating the results of said fitting operation to quantify the association between the said compound and the binding region computer model, thereby evaluating the ability of the said compound to associate with the said
10   binding region;

e) synthesizing said compound; and

f) contacting said compound with said molecule to determine the ability of said compound to activate or inhibit said molecule.

15   17. A method for identifying a ligand interaction with a molecule or molecule complex comprising a human serum albumin binding region selected from the group consisting of binding region IA, IA/IB, IA/IIA, IB, I/II; I/III; II/III, IIA, IIA/IIB, IIB, IIIA, IIIA/IIIB, IIIB and IIIB' comprising the steps of

a) constructing a computer model of the binding region defined by three-
20   dimensional structural binding coordinates wherein the root mean square deviation between said structural binding coordinates and the structural binding coordinates of the resulting complex within the binding region as set forth in Table II or III is not more than about 1.15 angstroms;

b) selecting a compound to be evaluated by a method selected from the
25   group consisting of (i) assembling molecular fragments into said compound, (ii) selecting a compound from a small molecule database, (iii) de novo ligand design of said compound, (iv) a compound obtained by modifying a compound with known binding affinity to a human serum albumin binding region; (v) a pharmaceutical or other compound as set forth in Tables I or II; (vi) a compound
30   obtained by modifying a known pharmaceutical compound, or active portion thereof, of human serum albumin

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c) employing computational means to perform a fitting program operation between computer models of the said compound to be evaluated and said binding region in order to provide an energy-minimized configuration of the said compound in the binding region;

5   d) evaluating the results of said fitting operation to quantify the association between the said compound and the binding region computer model, thereby evaluating the ability of the said compound to associate with the said binding region;

e) synthesizing said compound; and

10   f) contacting said compound with said molecule so as to determine the ability of said ligand interact with said molecule.

18. The method of claim 17 wherein the root mean square deviation is within about 2.5 angstroms.

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19. The method of claim 17 wherein the root mean square deviation is within about 3.0 angstroms.

20. A method of optimizing the binding of a compound to a human serum

20   albumin comprising a human serum albumin binding region selected from the group consisting of binding region IA, IA/IB, IA/IIA, IB, I/II; I/III; II/III, IIA, IIA/IIB, IIB, IIIA, IIIA/IIIB, IIIB and IIIB' comprising the steps of

a) constructing a computer model of the binding region defined by three-dimensional structural binding coordinates wherein the root mean square

25   deviation between said structural binding coordinates and the structural binding coordinates of the resulting complex within the binding region as set forth in Table II or III is not more than about 1.15 angstroms;

b) selecting a compound to be evaluated by a method selected from the group consisting of (i) assembling molecular fragments into said compound, (ii)

30   selecting a compound from a small molecule database, (iii) de novo ligand design of said compound, (iv) a compound obtained by modifying a compound

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with known binding affinity to a human serum albumin binding region; (v) a pharmaceutical or other compound as set forth in Tables I or II; (vi) a compound obtained by modifying a known pharmaceutical compound, or active portion thereof, of human serum albumin

5   c) employing computational means to perform a fitting program operation between computer models of the said compound to be evaluated and said binding region in order to provide an energy-minimized configuration of the said compound in the binding region;

           d) evaluating the results of said fitting operation to optimize the binding

10   characteristics of said compound to an albumin binding site.

           21. A method of producing a computer readable database comprising the three-dimensional molecular structural coordinates of one or more human albumin binding regions selected from the group consisting of the binding region

15   IA, IA/IB, IA/IIA, IB, I/II; I/III; II/III, IIA, IIA/IIB, IIB, IIIA, IIIA/IIIB, IIIB and IIIB', said method comprising a) obtaining three-dimensional structural coordinates defining said binding regions; and b) introducing said structural coordinates into a computer to produce a database containing the molecular structural coordinates of said binding regions.

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           22. A computer readable database produced by the method of Claim 21.

           23. The method of Claim 21 further comprising utilizing the structural representations stored in said database for predictive ADME.

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           24. A method of producing a computer readable database comprising a representation of a compound capable of binding one or more human albumin binding subdomains, said method comprising a) introducing into a computer program a computer readable database produced by claim 1; b) generating a

30   three-dimensional representation of one or more human albumin binding subdomains in said computer program; c) superimposing a three-dimensional

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model of at least one binding test compound on said representation of said one or more binding subdomains; d) assessing whether said test compound model fits spatially into one or more human serum albumin binding subdomains; and e) storing a structural representation of a compound that fits into one or more
5   human serum albumin binding subdomains.

        25.   A method of producing a computer readable database comprising a representation of a compound capable of binding one or more human albumin binding subdomains, said method comprising a) introducing into a computer
10   program a computer readable structural database comprising the three-dimensional molecular structural coordinates of one or more human albumin binding regions selected from the group consisting of the binding region IA, IA/IB, IA/IIA, IB, I/II; I/III; II/III, IIA, IIA/IIB, IIB, IIIA, IIIA/IIIB, IIIB and IIIB', said computer readable structural database produced by a method comprising obtaining three-
15   dimensional structural coordinates defining said binding regions and introducing said structural coordinates into a computer to produce a database containing the molecular structural coordinates of said binding regions; b) generating a three-dimensional representation of one or more human albumin binding subdomains in said computer program; c) superimposing a three-dimensional model of at
20   least one binding test compound on said representation of said one or more binding subdomains; d) assessing whether said test compound model fits spatially into one or more human serum albumin binding subdomains; and e) storing a structural representation of a compound that fits into one or more human serum albumin binding subdomains.
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        26.   A computer readable database produced by the method of Claim 25.

        27.   The method of Claim 25 further comprising utilizing the structural representations stored in said database for predictive ADME.
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28.   An isolated protein fragment comprising a human serum albumin binding subdomain selected from the group consisting of binding region IA, IA/IB, IA/IIA, IB, I/II; I/III; II/III, IIA/IIB, IIB, IIIA/IIIB, IIIB and IIIB'.

5   29.   A method of determining the binding affinity of a drug to a target human serum albumin binding subdomain selected from the group consisting of human binding subdomain selected from the group consisting of binding region IA, IA/IB, IA/IIA, IB; I/II; I/III; II/III; IIA/IIB, IIB, IIIA/IIIB; IIIB and IIIB' comprising the steps of isolating a protein fragment according to claim 28, introducing said 10   protein fragment to said drug in an amount and for a time sufficient to block the site on that drug that will bind to the target albumin binding subdomain, and then determining the level of human serum albumin binding of the drug following said introduction of said protein fragment in order to determine the binding affinity of the drug to the target albumin binding subdomain.

15   30.   The method of Claim 29 further comprising a step of using the determined binding affinity to the target binding subdomain to assess the likelihood that the drug will displace a molecule or compound at the target binding subdomain.

20   31.   A kit for performing the method of Claim 29 comprising an isolated protein fragment comprising a human serum albumin binding subdomain selected from the group consisting of binding region IA, IA/IB, IA/IIA, IB, I/II; I/III; II/III, IIA/IIB, IIB, IIIA/IIIB, IIIB and IIIB' in an amount sufficient to block the site on 25   a drug that would bind to a human serum albumin binding domain, a means to allow the introduction of the isolated fragment to a drug being assessed, and means to assess the binding of human serum albumin to the drug following introduction of the isolated fragment for a time sufficient to allow binding to take place.

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32. A method of assessing the binding affinity of a drug to a target human serum albumin binding subdomain selected from the group consisting of binding subdomain selected from the group consisting of binding region IA, IA/IB, IA/IIA, IB, I/II; I/III; II/III, IIA/IIB, IIB, IIIA/IIIB, IIIB and IIIB' comprising the steps of

5 obtaining a human serum albumin having a target binding subdomain that is blocked, introducing said blocked albumin to said drug and then determining the level of binding of the drug to the human serum albumin with a blocked target binding subdomain in order to assess the binding affinity of the drug to the target albumin binding subdomain.

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33. The method of Claim 32 further comprising a step of using the determined binding affinity to the target binding subdomain to assess the likelihood that the drug will displace a molecule or compound at the target binding subdomain.

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34. A kit for performing the method of Claim 32 comprising human serum albumin having a target binding subdomain that is blocked, a means to allow the introduction of the blocked human serum albumin to a drug being assessed, and means to assess the binding of the blocked human serum albumin to the drug

20 being assessed.